[redacted]

TECHNICAL MEMORANDUM
Sensitivity Testing of Area Source Parameters, Aggregation Assumptions, and Boundary Conditions

Earth Tech, Inc.

A set of sensitivity simulations have been conducted with the CALPUFF model to evaluate the response of model predictions in the Bridger and Fitzpatrick Class I areas to the methods of aggregation of the area sources and the values of the source parameters used in the SWWYTAF analysis. A second set of simulations were conducted examining the use of boundary cell emissions to simulate inflow conditions to the modeling domain.

The characteristics of the petroleum field area source emissions are not well known. Information such the magnitude of emissions from each individual well and even the location of the wells has a high degree of uncertainty. As a result, the well emissions were lumped into 20 km x 20 km grid squares for the SWWYTAF modeling. For more information on the petroleum emission estimates, see Volume 2 of the Emission Inventory report. An objective of the current analysis is to evaluate the sensitivity of the modeling results to the aggregation assumptions.

Figure 1 shows the locations of the PAW 20-km area sources as well as the Class I areas of interest (Bridger and Fitzpatrick Wilderness Areas). The aggregation test consisted of breaking each of the 76 20-km square area sources into a set of 5 x 5 4-km area sources (1900 4-km sources in all). The total pollutant emission rate per unit area was unchanged. The disaggregated sources had the same grid resolution as the computational grids used in the CALMET and CALPUFF simulations. As a result, the finer resolution 4-km emissions could produce different patterns of transport.

July 12, 1995 was selected for the simulation period because it produced high impacts from the petroleum sources in the Class I areas in the original simulations. New 24-hour simulations were conducted with the original 76 area sources and the disaggregated 1900 sources. The gridded receptor option was turned on (producing 116 x 100 gridded receptors, in addition to the 232 discrete receptors used in the original runs). The 24-hour average concentrations of NO_2 for each case are presented in Figures 2 and 3. The spatial patterns of NO_2 concentrations and the magnitudes of the peak concentrations produced in the Class I areas are very similar in the two simulations. Similar results are presented in Figures 4 and 5 for 24-hour average values of NO_3. These results indicate a general insensitivity to the aggregation of the petroleum well emissions into the 20-km cells in the original inventory, suggesting the use of 76 20-km area sources to characterize these sources is adequate.

As noted above, individual wells were lumped into 20 km square area sources in the base case simulations. Two characteristics of an area source that must be estimated are the effective height and the initial vertical distribution of the emissions. Given the nature of the well emissions (near-surface, low buoyancy releases), a release height of 10 meters and initial σ_z of 25 meters were used in the initial CALPUFF simulations. These values, although somewhat arbitrary, are based on the general characteristics of the source. It is hoped that the concentration predictions are not sensitive to these assumptions. A strong sensitivity would indicate the need to better characterize the emissions in order to obtain accurate modeling results.

In the current sensitivity tests, the emission height was doubled (to 20 meters) and halved (to 5 meters) in one set of two tests (with the initial σ_z set to the original value of 25 meters). Two additional simulations were then conducted with the emission height at 10 meters, but the initial σ_z doubled (50 meters) and halved (12.5 meters). All other parameters were unchanged from the original, base-case runs (i.e., 20 km square area sources were used in all the runs).

The 24-hour averaged NO_2 results of the source height tests are shown in Figures 6 and 7. The NO_2 results for the initial σ_z tests are shown in Figures 8 and 9. These results should be compared to the base case results in Figure 2. A similar set of plots are presented for NO_3 in Figures 10-13, for comparison to the base case result in Figure 4.

The conclusion is that the predicted concentrations in the Bridger and Fitzpatrick Class I areas are not sensitive to the source height or initial σ_z assumption for the petroleum (area) sources being considered in the SWWYTAF analysis. This suggests the original set of assumptions of 10 meter release heights and initial σ_z values of 25 meters are adequate.

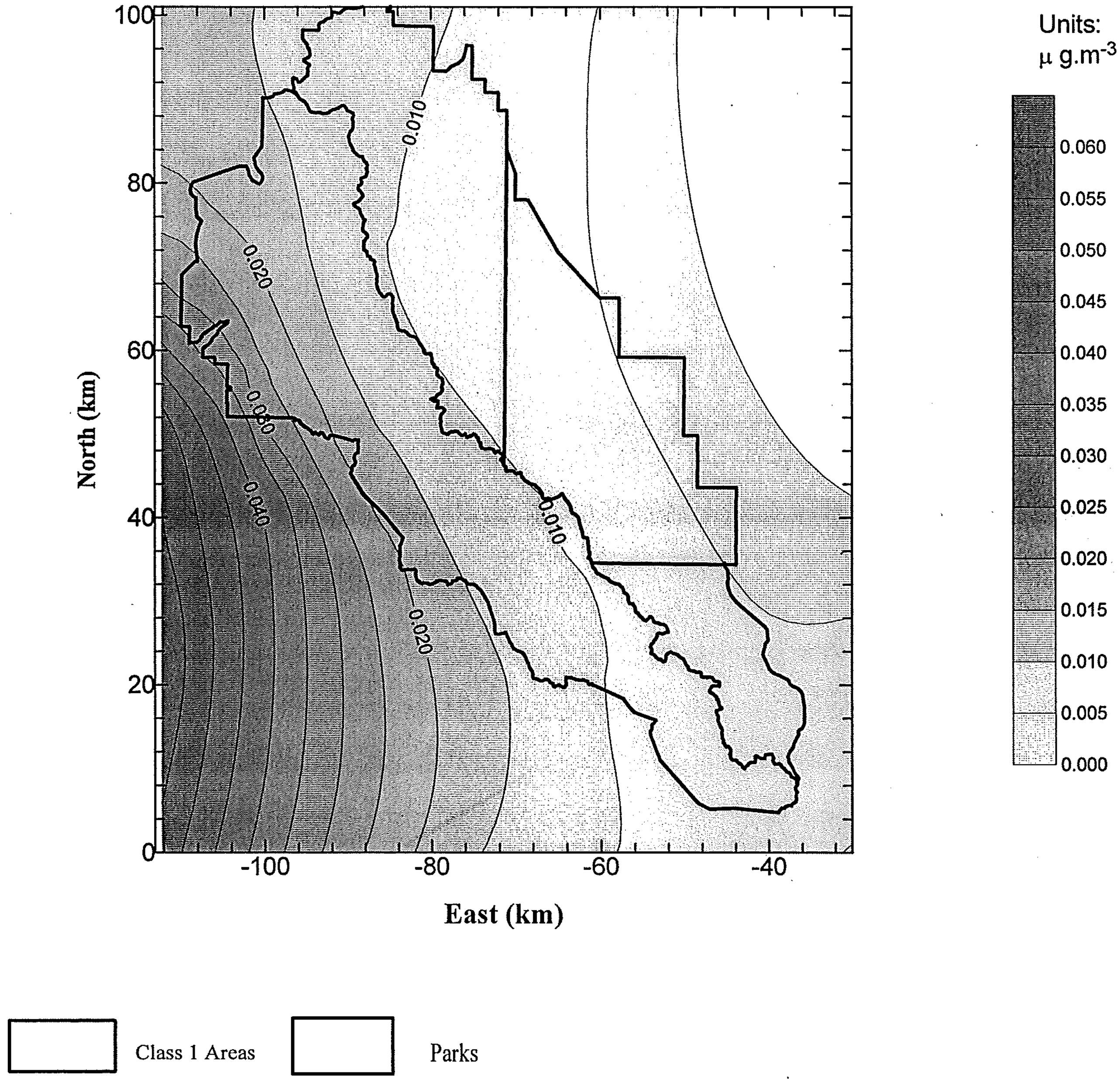
The final tests conducted involved the placement of volume sources in the boundary cells of the CALPUFF computational domain in order to simulate the inflow of pollutants from outside the domain. The volume sources were located along the southern boundary of the domain, one per computational grid cell (116 in all). An effective release height of 10 meters was used. Because of the large distance to the Class I areas, nominal values of initial σ_y of 50 meters were used. In the vertical, the CALPUFF option to use a uniformly vertical distribution was selected. This allows the "background" pollutant concentrations in the inflow air to be uniformly spread throughout the mixed layer. For testing purposes, an unit emission rate (1 g/s) was assigned to each volume source. The pollutant modeled was SO_2. Chemical conversion and wet/dry deposition processes were modeled, as in the base case simulations.

The patterns of SO_2 concentrations for one-hour averages and 24-hour averages are shown in Figures 14 and 15. The results suggest in those border areas with inflow winds, the residence time of SO_2 is sufficient to transport some pollutant material into the Class I area (see Figure 14), although the significance of the low concentrations predicted will depend on the strength of the boundary source. Averaged over 24-hours (see Figure 15), the border regions show a reasonable spatial distribution, suggesting the use of volume sources in the boundary cells is a feasible method to simulate inflow boundary conditions. In an operational application, the time-varying volume source option should be used, to allow the effective emission rates to vary with the meteorological conditions in order to obtain the desired background concentration in the boundary cell.

Fig. 2

PAW-Source Related [NO2] in Bridger Area

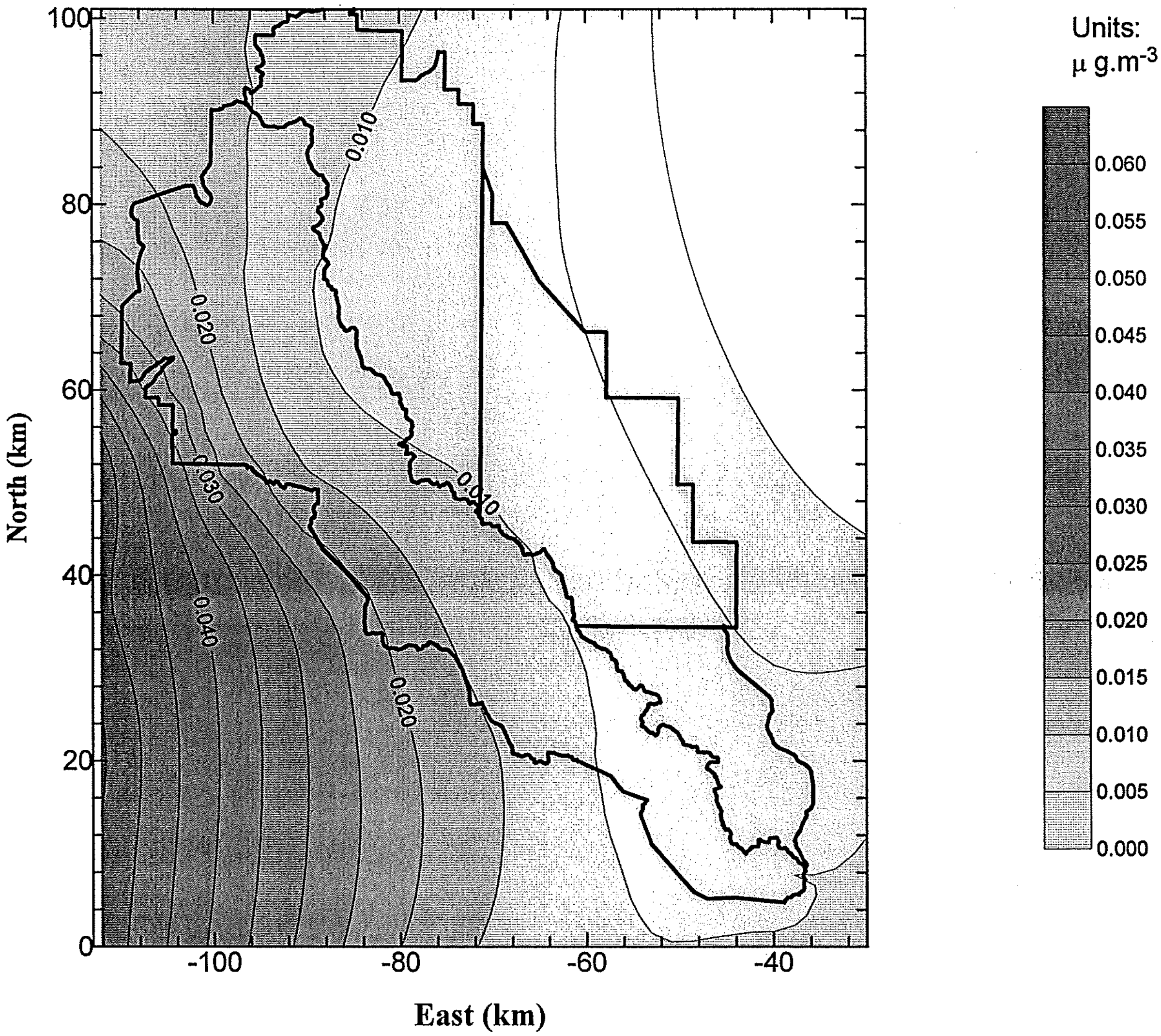
Original Source Parameters on July 12, 1995



e:/projects/swwytaf/9901/1932423p.srf

Fig. 3 **PAW-Source Related [NO2] in Bridger Area**

4km-Grid Source Parameters on July 12, 1995



Class 1 Areas Parks

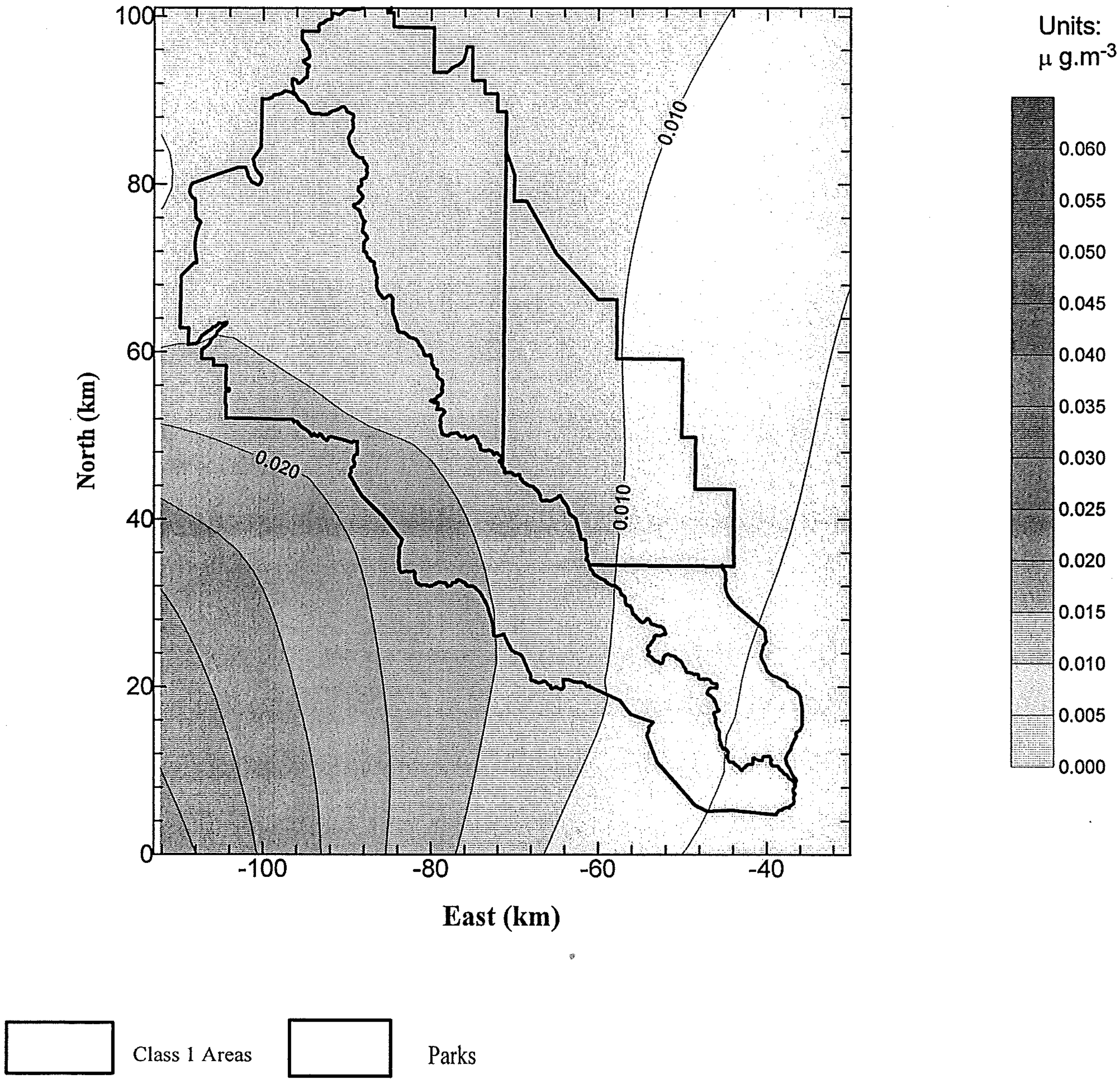
e:/projects/swwytaf/9901/1932423a.srf

SOLVAY2016_1.4_002044

Fig. 4

PAW-Source Related [NO3] in Bridger Area

Original Source Parameters on July 12, 1995



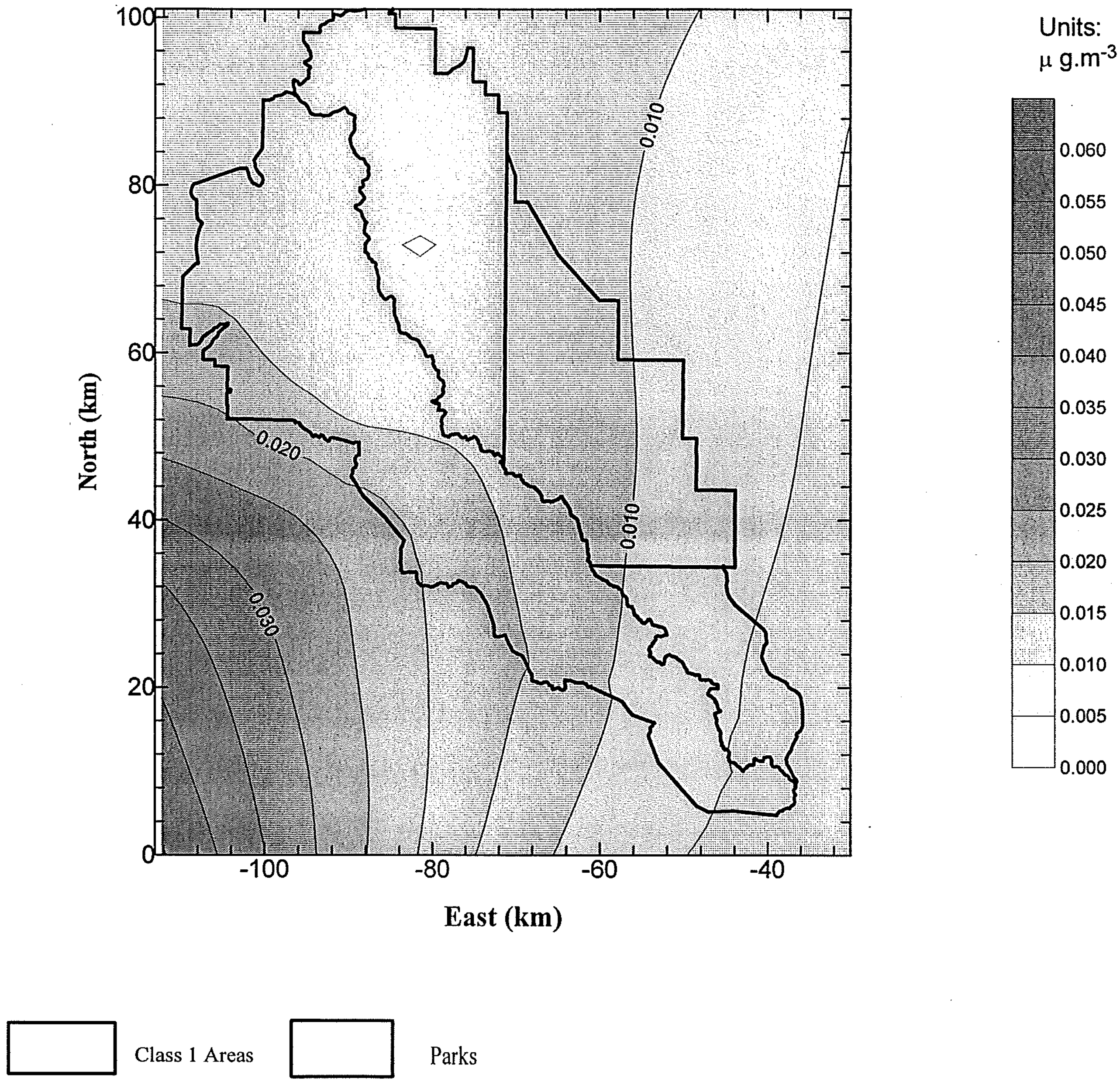
e:/projects/swwytaf/9901/1932423u.srf

SOLVAY2016_1.4_002045

Fig. 5

PAW-Source Related [NO3] in Bridger Area

4km-Grid Source Parameters on July 12, 1995



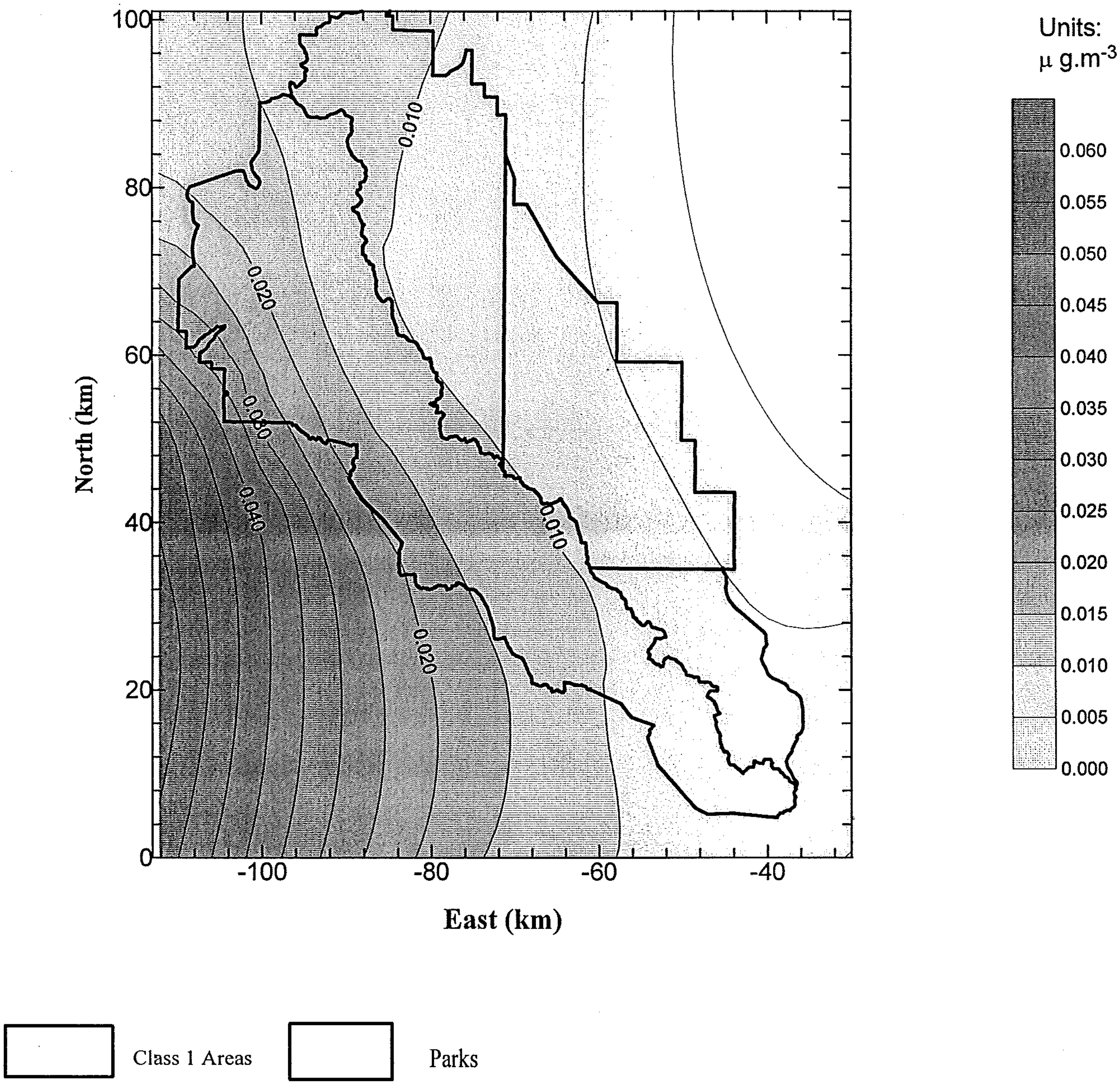
e:/projects/swwytaf/9901/1932423b.srf

SOLVAY2016_1.4_002046

Fig. 6

PAW-Source Related [NO2] in Bridger Area

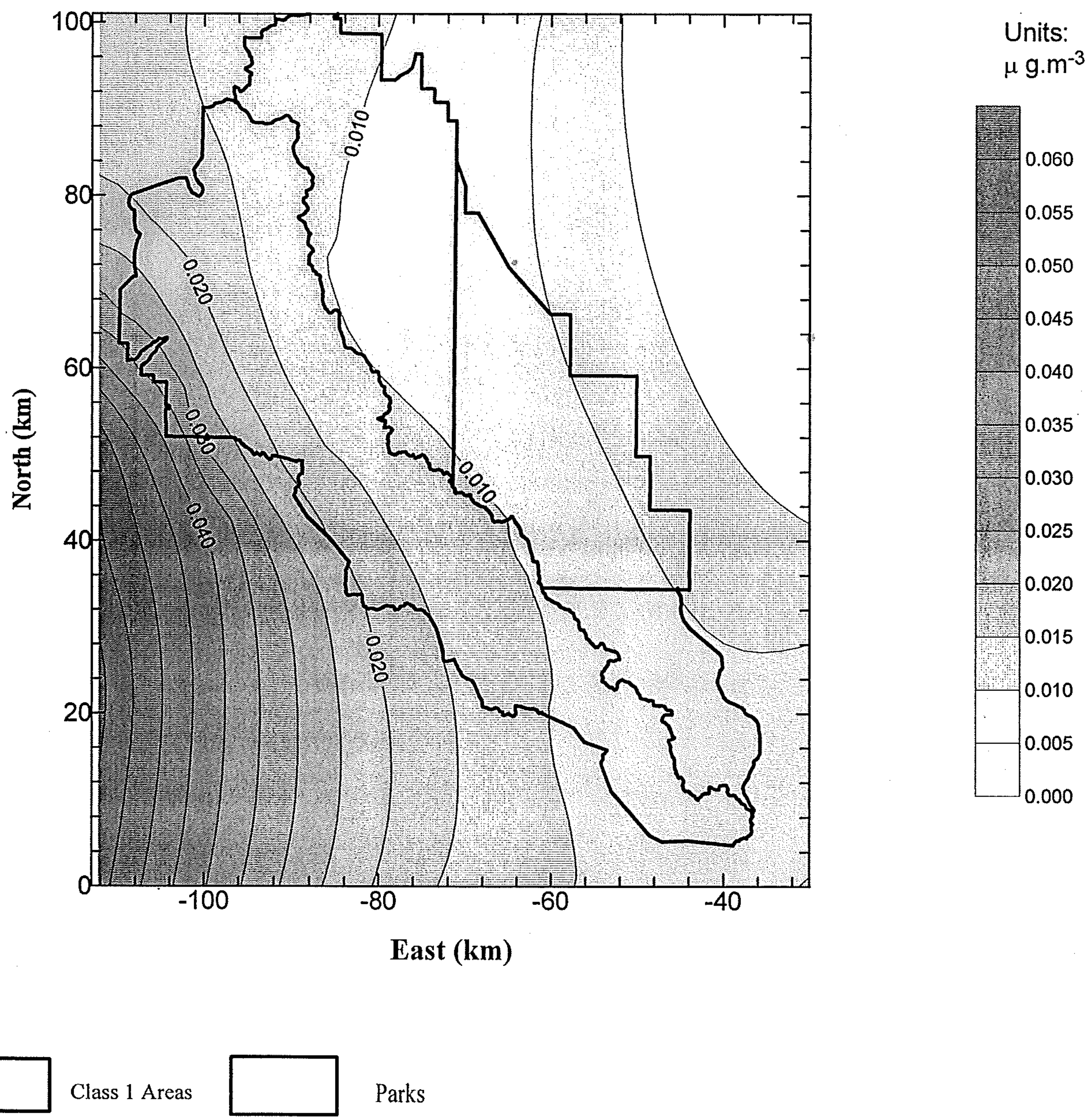
Half-Height Source Parameters on July 12, 1995



e:/projects/swwytaf/9901/1932423q.srf

Fig. 7 **PAW-Source Related [NO2] in Bridger Area**

Double-Height Source Parameters on July 12, 1995



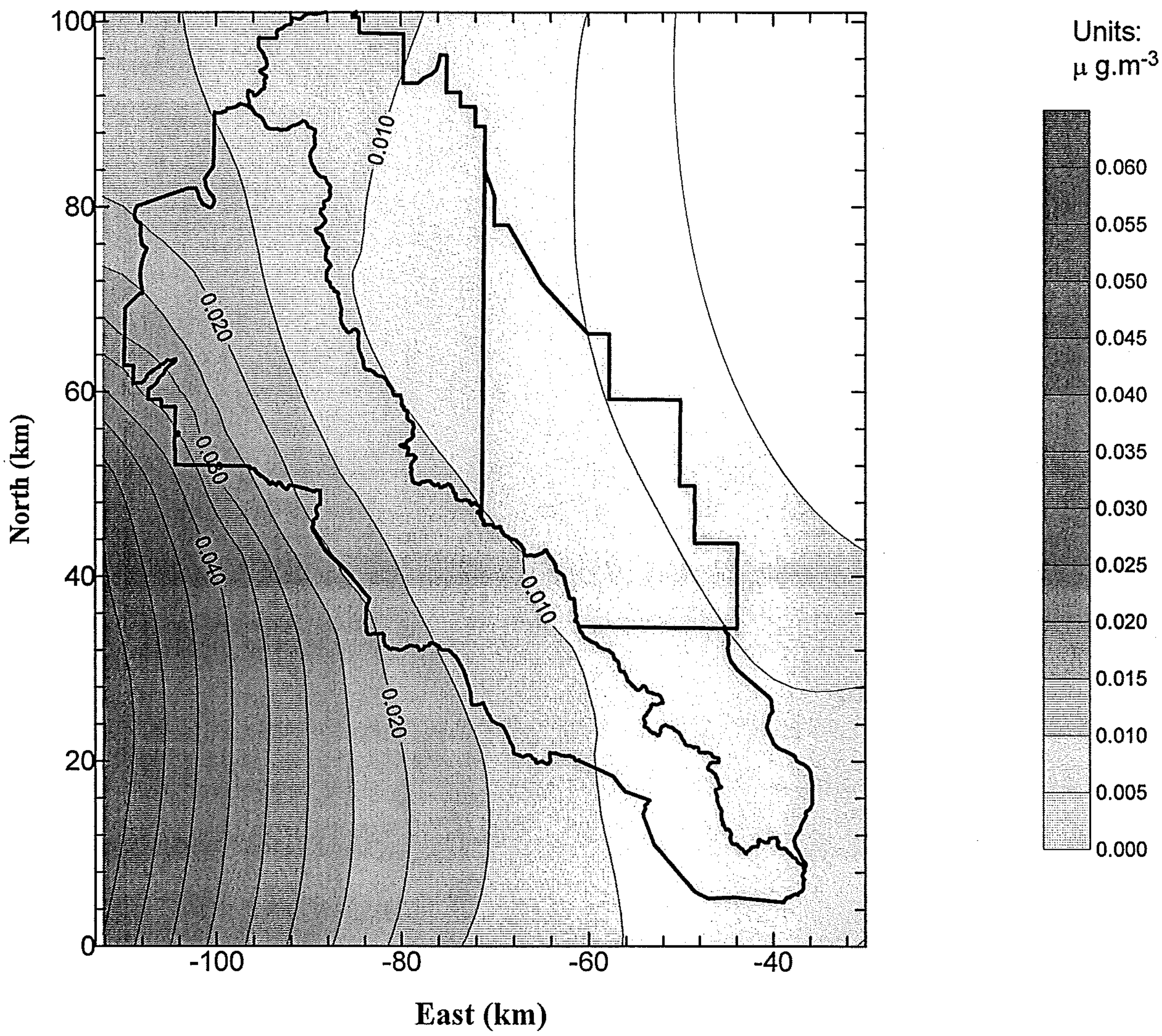
e:/projects/swwytaf/9901/1932423r.srf

SOLVAY2016_1.4_002048

Fig. 8

PAW-Source Related [NO2] in Bridger Area

Half-SigmaZ Source Parameters on July 12, 1995



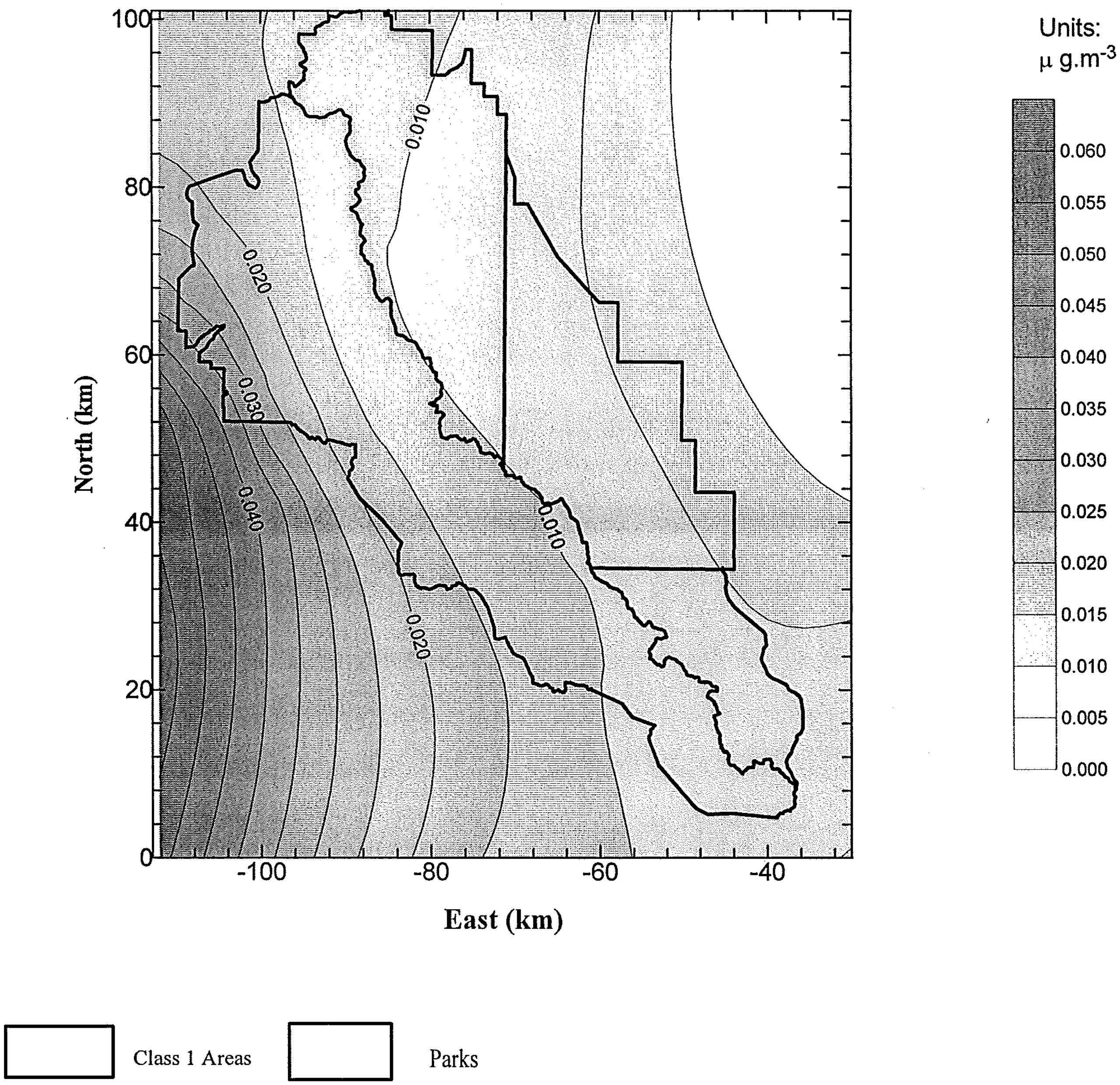
Class 1 Areas

Parks

e:/projects/swwytaf/9901/1932423s.srf

Fig.9 **PAW-Source Related [NO2] in Bridger Area**

Double-SigmaZ Source Parameters on July 12, 1995



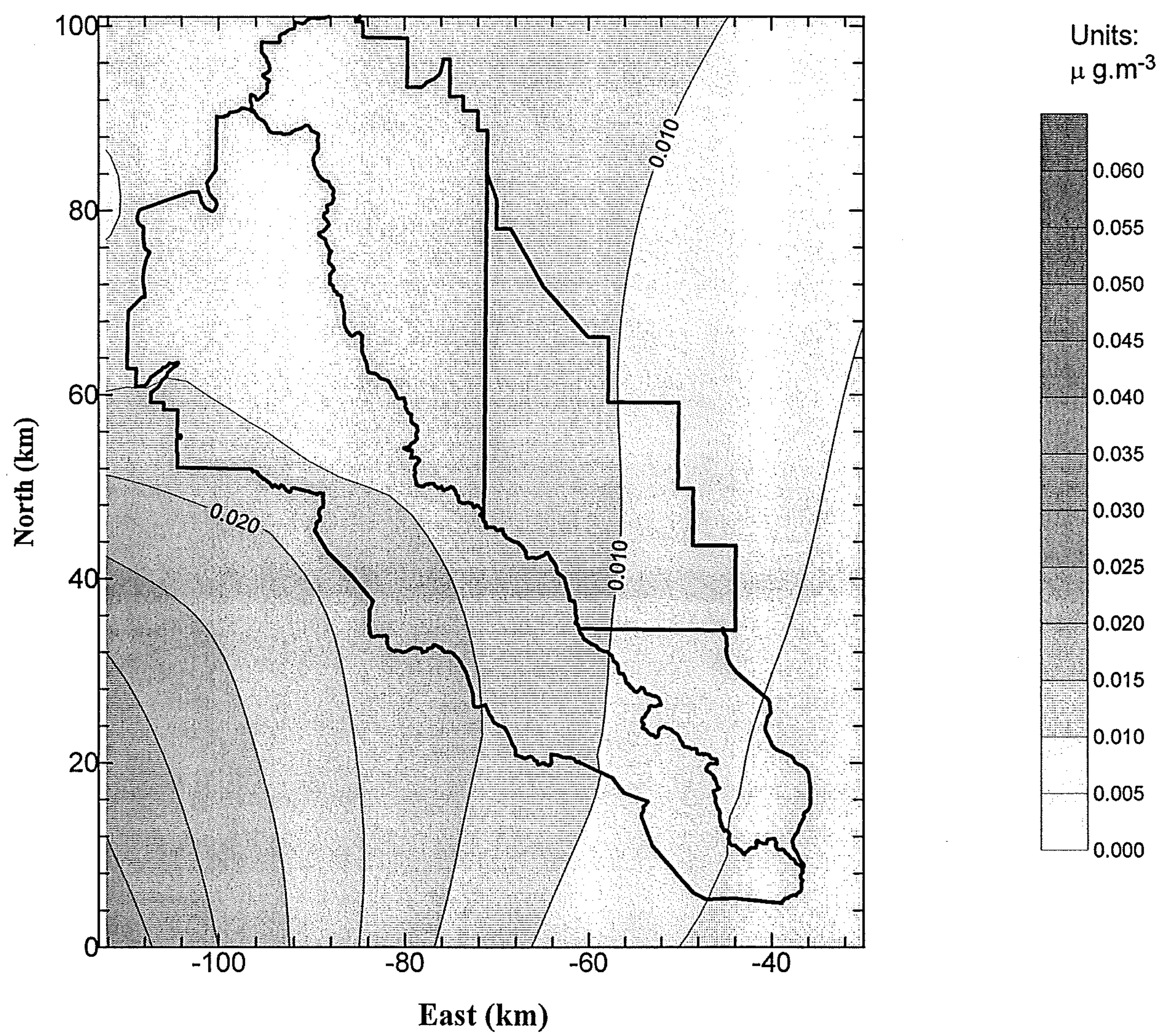
e:/projects/swwytaf/9901/1932423t.srf

SOLVAY2016_1.4_002050

Fig. 10

PAW-Source Related [NO3] in Bridger Area

Half-Height Source Parameters on July 12, 1995



Class 1 Areas

Parks

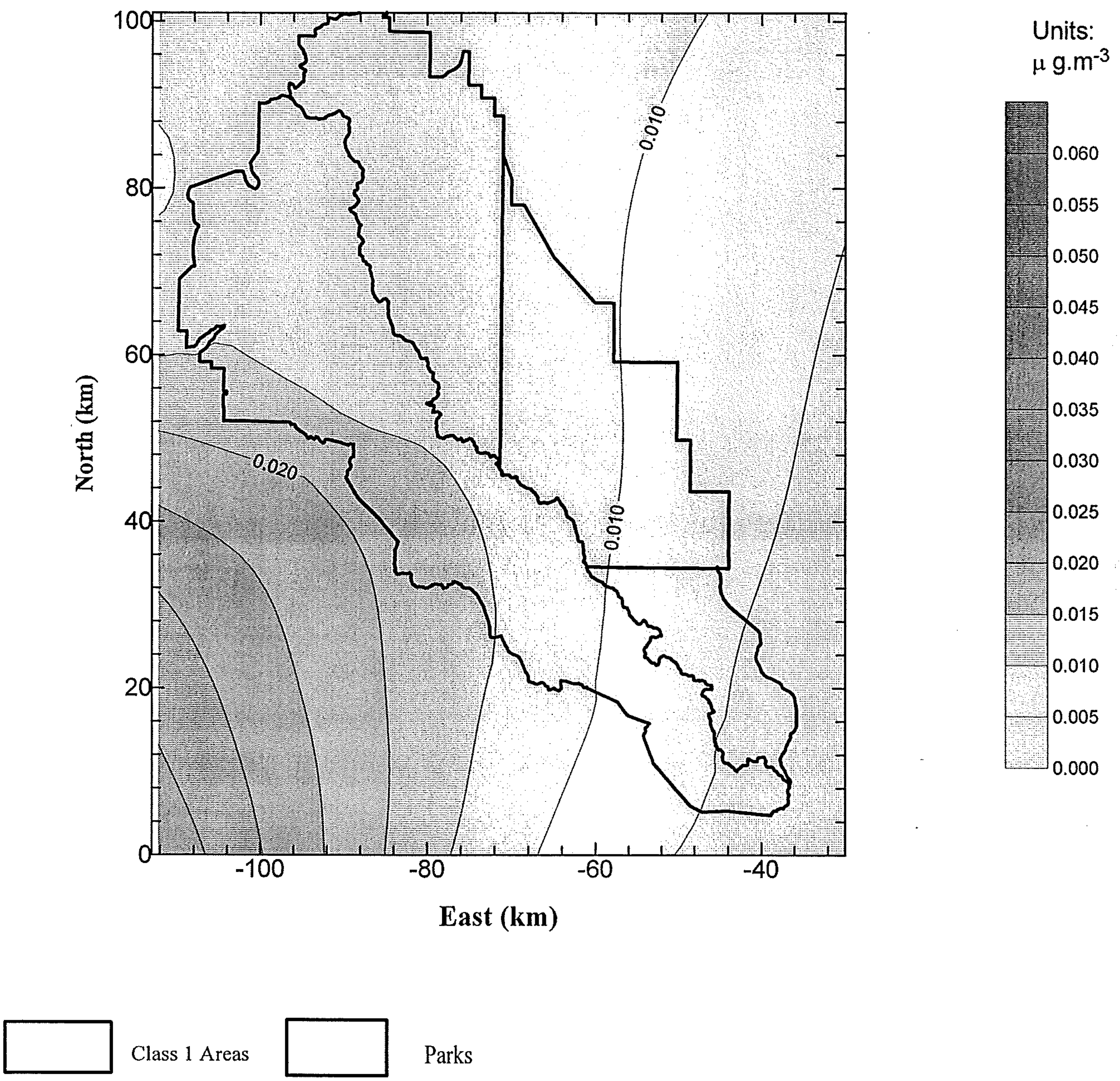
e:/projects/swwytaf/9901/1932423v.srf

SOLVAY2016_1.4_002051

Fig. 11

PAW-Source Related [NO3] in Bridger Area

Double-Height Source Parameters on July 12, 1995



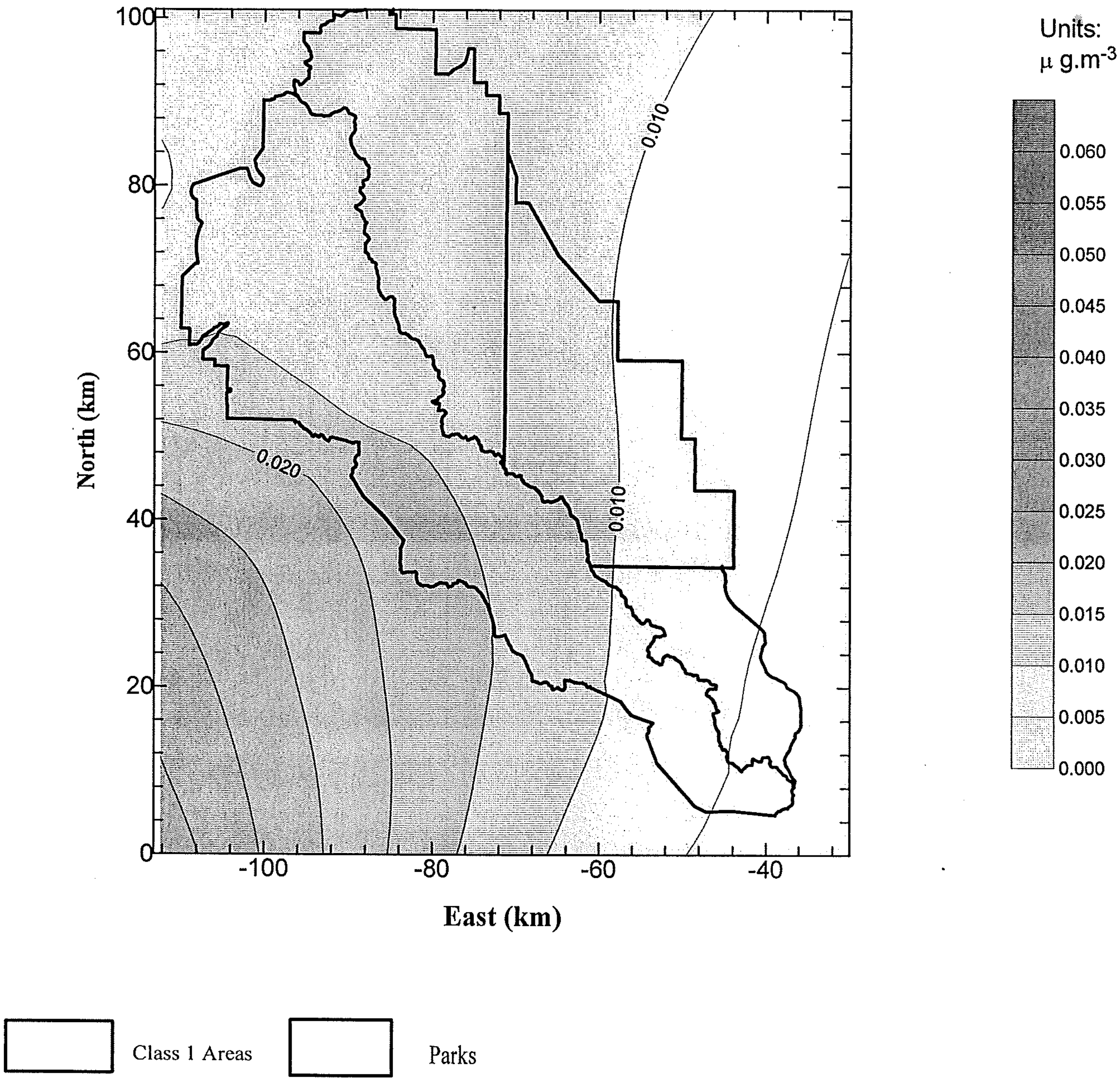
e:/projects/swwytaf/9901/1932423w.srf

SOLVAY2016_1.4_002052

Fig. 12

PAW-Source Related [NO3] in Bridger Area

Half-SigmaZ Source Parameters on July 12, 1995



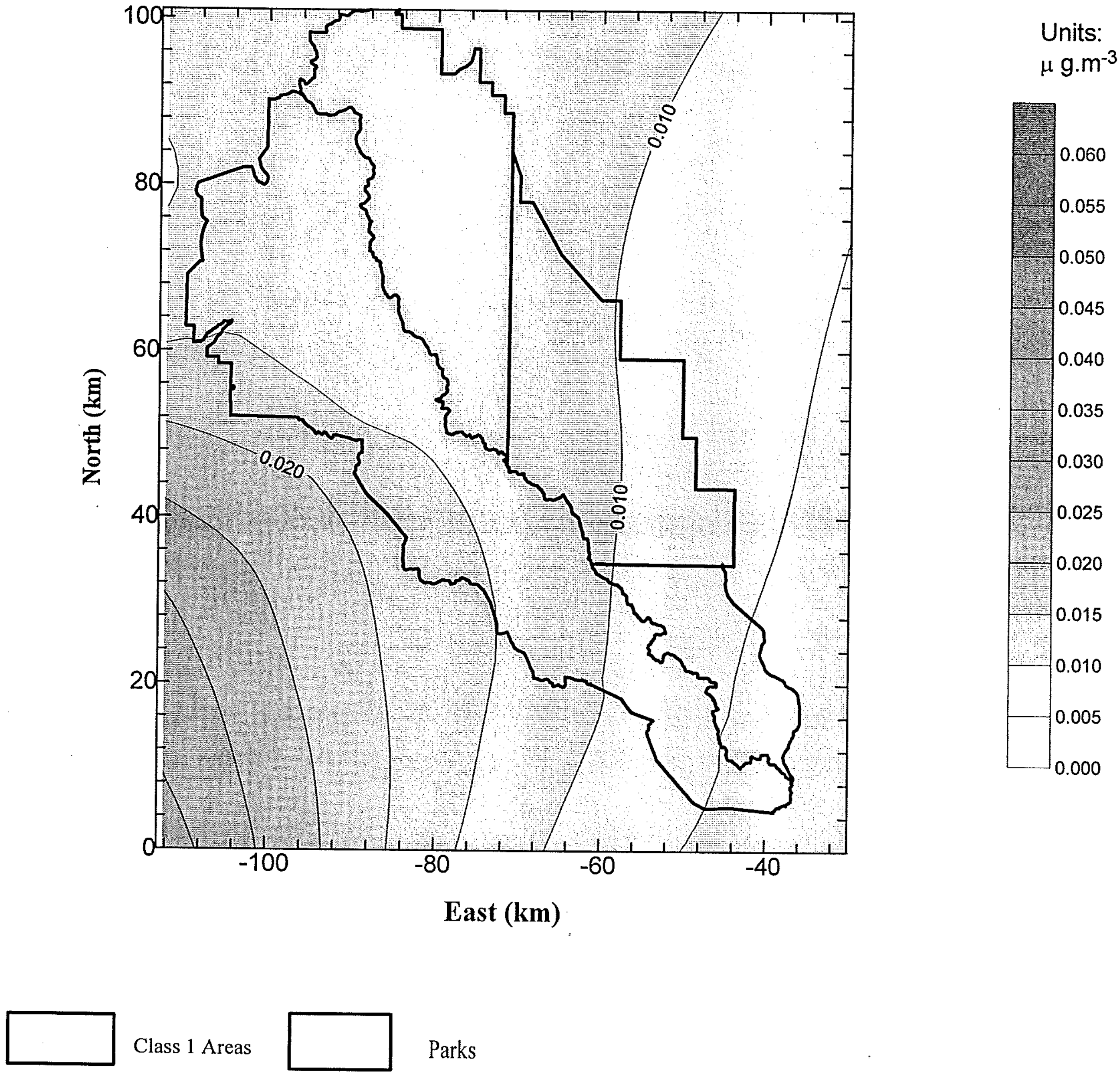
e:/projects/swwytaf/9901/1932423x.srf

SOLVAY2016_1.4_002053

Fig. 13

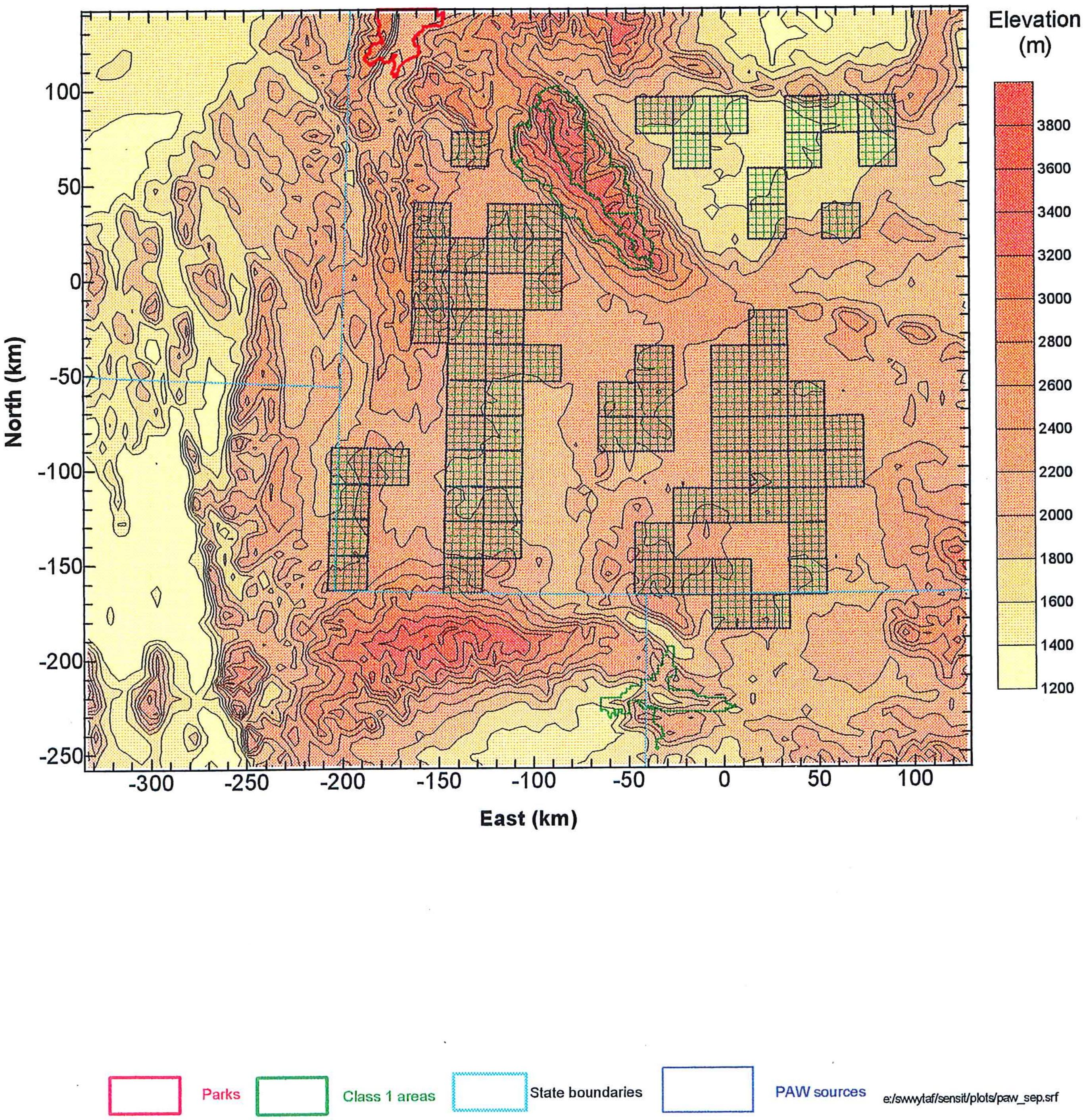
PAW-Source Related [NO3] in Bridger Area

Double-SigmaZ Source Parameters on July 12, 1995



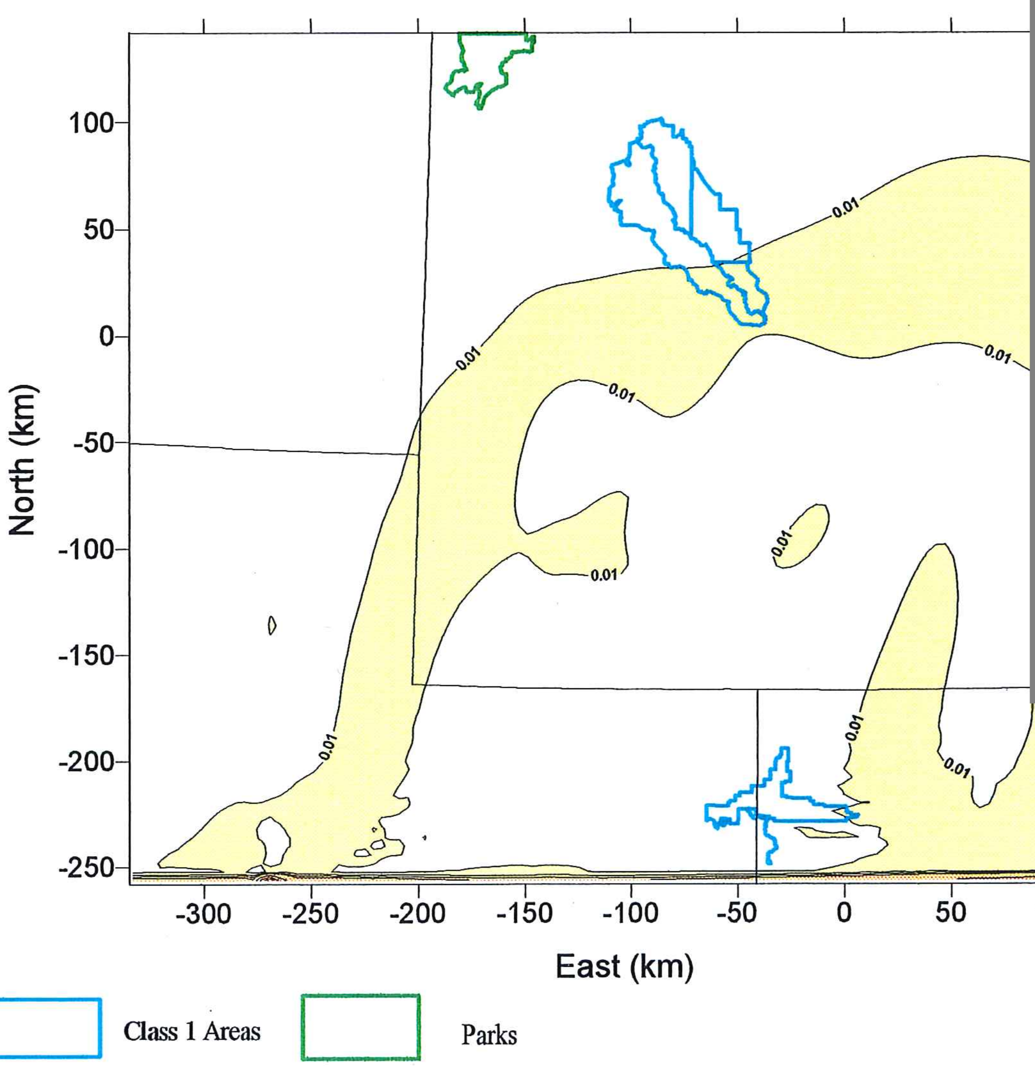
e:/projects/swwytaf/9901/1932423y.srf

Figure 1. Revised PAW 20-km Emission Source Locations and 4-km Emission Source Locations Used in Sensitivity Runs



SOLVAY2016_1.4_002055

Fig. 14. 1-Hr Averaged [SO2] at 5PM on July 12, 1995

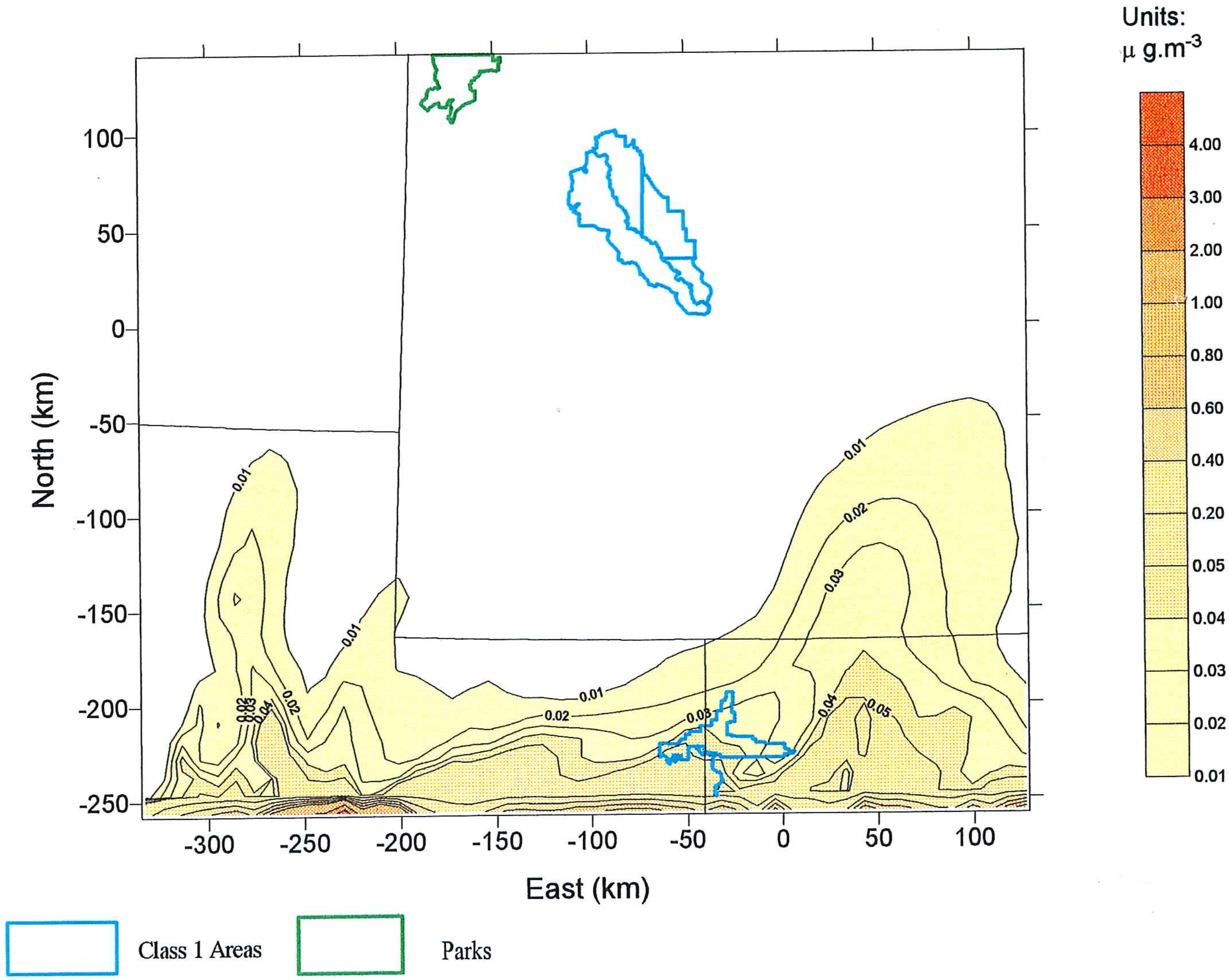


e:/projects/swwy

SOLVAY2016_1.4_002056

Fig. 15

24-Averaged [SO2] on July 12, 1995



e:/projects/swwytaf/9901/so2193.srf

SOLVAY2016_1.4_002057